

Lattice Discretization in Quantum Scattering

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Abstract

The utility of lattice discretization technique is demonstrated for solving nonrelativistic quantum scattering problems and specially for the treatment of ultraviolet divergences in these problems with some potentials singular at the origin in two and three space dimensions. This shows that lattice discretization technique could be a useful tool for the numerical solution of scattering problems in general. The approach is illustrated in the case of the Dirac delta function potential.

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The technique of discretization on lattice (hereafter called lattice technique) [1, 2, 3] has been successfully used to deal with ultraviolet divergences in gauge field theoretic problems in perturbative expansion, specially those in quantum electrodynamics (QED) and quantum chromodynamics (QCD). These ultraviolet divergences in perturbative quantum field theory can be eliminated by lattice technique to yield a scale. Except in some simple cases the lattice-regularized perturbative series can not be summed up and this makes it difficult to draw conclusions about the full solution. The renormalization group (RG) equations [4, 5], on the other hand, yield many general properties of the full solution from the lattice-regularized results of the perturbative expansion.

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The lattice technique represents a mathematical trick, which removes the ultraviolet divergences by introducing a cutoff in a regularized Green function. As with any regulator, it is removed after renormalization. The physical observables are then obtained in the continuum limit, where the lattice spacing is taken to be zero.

Ultraviolet divergences also appear in the nonrelativistic quantum scattering problems for potentials with certain singular behavior at short distances [6, 7, 8, 9] in two and three dimensions. In one dimension these divergences are absent. We show that the application of the lattice technique to these potential models leads to a scale and finite physical observables after the continuum limit is taken by the usual renormalization procedure. The present work is written in a pedagogic style so that it clarifies all the subtleties of lattice technique in a simple nonrelativistic problem and should serve as an introduction to the study of lattice technique in a complicated field theoretic problem.

Recently, there have been discussions on renormalization in configuration [8] and momentum [6, 7, 9] spaces for potential scattering with the Dirac delta, contact, or zero-range potential. In this work the lattice technique is used for potential scattering with delta potential in two and three dimensions. In both cases there are ultraviolet divergences. In the two dimensional case the divergence is logarithmic in nature, whereas in the three-dimensional case it is linear. The lattice-regularized result is finally renormalized and the RG equation written.

The present potential scattering problem permits analytic solution and is infinitely simpler than gauge field theories of QED and QCD where the lattice technique is usually applied. Hence the present study will allow us to understand the subtleties of this approach. In gauge field theories particles can be spontaneously created and destroyed and the discretization is done in the four-dimensional Euclidean space. In potential scattering particle number is conserved and we directly discretize the time-independent Schrödinger equation for relative motion in three-dimensional Euclidean space.

The present analytic investigation with delta potential shows the subtleties of the lattice technique and demonstrates that this approach can be used for a numerical solution of non-relativistic quantum scattering problems in general, not only for two particles but for several particles. In this analytic study we calculate the nonrelativistic Green function and the t matrix on the lattice. The numerical study remains one to be attempted in the future.

There is another interest to study the nonrelativistic scattering with delta potential in two dimensions. This problem can be considered to be a good model of the ultraviolet structure and high energy behavior of $\lambda\phi^4$ field theory [5, 8, 9]. Both problems have ultraviolet logarithmic divergences, require regularization, are perturbatively renormalizable, collapse for attractive

interaction but are asymptotically free, etc.

We discuss S -wave potential scattering with the delta potential. The partial-wave Lippmann-Schwinger equation for the scattering amplitude $T(p, q, k^2)$ in \mathcal{D} dimensions at c.m. energy k^2 is given by

$$T(p', p, k^2) = V(p', p) + \int d^{\mathcal{D}}q V(p', q) G(q; k^2) T(q, p, k^2), \quad (1)$$

with the free Green function $G(q; k^2) = (k^2 - q^2 + i0)^{-1}$, in units $\hbar = 2m = 1$, where m is the reduced mass. The integral in Eq. (1) is over the relevant S -wave phase space, e.g., we take $d^3q \equiv 4\pi q^2 dq$ and $d^2q \equiv 2\pi q dq$ with q varying from 0 to ∞ . For the delta potential $V(p', p) = \lambda$, and

$$T(p', p, k^2) = [\lambda^{-1} - I(k)]^{-1}, \quad (2)$$

with $I(k) = \int d^{\mathcal{D}}q G(q; k^2)$. The integral $I(k)$ possesses ultraviolet divergence for $\mathcal{D} > 1$. For $\mathcal{D} = 3$ (2) this divergence is linear (logarithmic) in nature. Finite result for the t matrix of Eq. (2) can be obtained only if λ^{-1} also diverges in a similar fashion and cancels the divergence of $I(k)$.

The solution of the problem can be achieved by discretizing the full Schrödinger equation on lattice and finding its solution numerically. Instead, as this problem permits analytic solution, we discretize the free Schrödinger equation on lattice and evaluate the lattice-regularized free Green function. With the lattice-regularized Green function the ultraviolet divergences are avoided. In contrast to the lattice discretization of gauge field theories, where one works in terms of Lagrangian densities and path integrals [2, 3], in the present problem it is convenient to work in terms of the following time-independent Schrödinger equation for relative motion

$$\nabla_{\mathbf{r}}^2 \phi(\mathbf{r}) + k^2 \phi(\mathbf{r}) = 0, \quad (3)$$

where the space vector $\mathbf{r} \equiv (x_j), j = 1, \dots, \mathcal{D}$. The present mathematical treatment is much simpler than, but similar to, that in field theory [2]. For our purpose we consider the \mathcal{D} -dimensional lattice of spacing a . The transition from the continuum to the discrete lattice is then effected by making the following substitutions [1, 2]

$$\begin{aligned} x_j &\rightarrow \mathbf{n}a \equiv n_j a, j = 1, \dots, \mathcal{D}, \\ \phi(\mathbf{r}) &\rightarrow \phi_{\mathbf{n}} \equiv \phi(\mathbf{n}a) \\ \nabla_{\mathbf{r}}^2 \phi(\mathbf{r}) &\rightarrow a^{-2} \sum_{j=1}^{\mathcal{D}} \left[\phi(\mathbf{n}a + \hat{\mathbf{j}}a) + \phi(\mathbf{n}a - \hat{\mathbf{j}}a) - 2\phi(\mathbf{n}a) \right]. \end{aligned}$$

Here the space coordinate is discretized by $\mathbf{r} = \mathbf{n}a$ and $\hat{\mathbf{j}}$ is the unit vector in direction j . The individual component n_j assumes only a finite number N of independent values. Outside this

range the lattice is assumed to be periodic, so that the n th site can be identified with the $(n + N)$ th site. The active part of the lattice has $N^{\mathcal{D}}$ sites.

After discretization, the Schrödinger equation (3) becomes the matrix equation

$$\sum_{\mathbf{m}} K_{\mathbf{nm}} \phi_{\mathbf{m}} = 0, \quad (4)$$

where

$$K_{\mathbf{nm}} = a^{-2} \sum_{j=1}^{\mathcal{D}} \left[\delta_{\mathbf{n}+\hat{\mathbf{j}},\mathbf{m}} + \delta_{\mathbf{n}-\hat{\mathbf{j}},\mathbf{m}} + (a^2 k_j^2 - 2) \delta_{\mathbf{n},\mathbf{m}} \right]. \quad (5)$$

Comparing Eqs. (3) and (4) we realize that $K_{\mathbf{nm}}$ is the discretized version of the operator $(\nabla_{\mathbf{r}}^2 + k^2)$. Hence, the free Green function is the inverse of this operator, defined by

$$\sum_{\mathbf{m}} K_{\mathbf{nm}} (K^{-1})_{\mathbf{ml}} = \delta_{\mathbf{nl}}. \quad (6)$$

This inverse operator can be evaluated analytically by working in momentum space where the \mathcal{D} -dimensional Kröner δ functions are represented as

$$\delta_{\mathbf{nm}} = \left(\prod_{l=1}^{\mathcal{D}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) e^{i\tilde{\mathbf{q}} \cdot (\mathbf{n}-\mathbf{m})}, \quad (7)$$

where $\tilde{\mathbf{q}}$ is a dimensionless wave number defined by $\tilde{\mathbf{q}} = a\mathbf{q}$ with components \tilde{q}_j . The integration is restricted to the first Brillouin zone $-\pi \leq \tilde{q}_l \leq \pi$. In the continuum limit one has the following relations for the phase spaces

$$\begin{aligned} \int d^{\mathcal{D}} q &\equiv \lim_{a \rightarrow 0} \left(\prod_l^{\mathcal{D}} \frac{1}{a^{\mathcal{D}}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) \\ &= \lim_{a \rightarrow 0} \left(\prod_l^{\mathcal{D}} \int_{-\pi/a}^{\pi/a} \frac{dq_l}{(2\pi)^3} \right). \end{aligned} \quad (8)$$

Using the Fourier representation (7), the matrix K can be written as

$$\begin{aligned} K_{\mathbf{nm}} &= a^{-2} \left(\prod_{l=1}^{\mathcal{D}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) e^{i\tilde{\mathbf{q}} \cdot (\mathbf{n}-\mathbf{m})} \sum_{j=1}^{\mathcal{D}} \left[e^{i\tilde{\mathbf{q}} \cdot \hat{\mathbf{j}}} + e^{-i\tilde{\mathbf{q}} \cdot \hat{\mathbf{j}}} + (a^2 k_j^2 - 2) \right], \\ &= a^{-2} \left(\prod_{l=1}^{\mathcal{D}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) e^{i\tilde{\mathbf{q}} \cdot (\mathbf{n}-\mathbf{m})} \left[(a^2 k^2 - 2\mathcal{D}) + \sum_{j=1}^{\mathcal{D}} 2 \cos \tilde{q}_j \right]. \end{aligned} \quad (9)$$

The inverse of the matrix K is now determined by

$$(K^{-1})_{\mathbf{nm}} = a^2 \left(\prod_{l=1}^{\mathcal{D}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) e^{i\tilde{\mathbf{q}} \cdot (\mathbf{n}-\mathbf{m})} \left[(a^2 k^2 - 2\mathcal{D}) + \sum_{j=1}^{\mathcal{D}} 2 \cos \tilde{q}_j \right]^{-1}. \quad (10)$$

This result leads to the following lattice-regularized outgoing-wave Green function

$$G_R(q, a; k^2) = a^2 \left[(a^2 k^2 - 2\mathcal{D}) + \sum_{j=1}^{\mathcal{D}} 2 \cos \tilde{q}_j + i0 \right]^{-1}. \quad (11)$$

With this Green function there is no ultraviolet divergence for $a \neq 0$. The imaginary part of this Green function guarantees unitarity for outgoing-wave scattering. In the limit $a \rightarrow 0$, the regularized Green function reduces to the free Green function: $\lim_{a \rightarrow 0} G_R(q, a; k^2) = G(q; k^2)$.

Using the lattice-regularized Green function (11), the t matrix (2) can be rewritten as

$$T(k, \lambda(a), a) = [\lambda^{-1}(a) - I_R(k, a)]^{-1}, \quad (12)$$

where

$$\begin{aligned} I_R(k, a) &\equiv \int d^{\mathcal{D}} q G_R(q, a; k^2) \\ &= a^{(2-\mathcal{D})} \left(\prod_{l=1}^{\mathcal{D}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) \left[(a^2 k^2 - 2\mathcal{D}) + \sum_{j=1}^{\mathcal{D}} 2 \cos \tilde{q}_j + i0 \right]^{-1}, \end{aligned} \quad (13)$$

is a convergent integral for a finite lattice spacing a . In Eq. (12) the redundant momentum labels p, p' of the t matrix have been suppressed, and the explicit dependences of the t matrix on a and $\lambda(a)$ have been introduced. As $a \rightarrow 0$, however, this integral develops the original ultraviolet divergence. Explicitly,

$$\lim_{a \rightarrow 0} I_R(k, a) = -[c/a + 2\pi^2 i k], \mathcal{D} = 3, \quad (14)$$

$$\lim_{a \rightarrow 0} I_R(k, a) = 2\pi \ln(ak) - i\pi^2, \mathcal{D} = 2, \quad (15)$$

where

$$c \equiv \left(\prod_{l=1}^{\mathcal{D}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) \left[6 - \sum_{j=1}^3 2 \cos \tilde{q}_j \right]^{-1}, \quad (16)$$

is a real finite definite integral.

Finite results for physical magnitudes, as $a \rightarrow 0$, are obtained from Eq. (12) if the coupling λ is also replaced by the so called bare coupling $\lambda(a)$ as in this equation. The bare coupling can, for example, be defined by

$$\lambda^{-1}(a) = -[c/a + 2\pi^2 \Lambda_0], \mathcal{D} = 3, \quad (17)$$

$$= 2\pi [\ln(a\Lambda_0)], \mathcal{D} = 2, \quad (18)$$

where Λ_0 is the physical scale of the problem and characterizes the strength of the interaction. The quantities $\lambda^{-1}(a)$ of Eqs. (17) and (18) have the appropriate divergent behavior, as $a \rightarrow 0$, and cancel the divergent part of $I_R(k, a)$ in Eq. (12).

Regarding the lattice merely as an ultraviolet regulator or cutoff (lattice spacing a), finally, we must take the continuum limit: $a \rightarrow 0$. For the present delta potential this limit can be taken analytically. In a general problem the limit has to be taken numerically. Both ways are illustrated below. After this limit is taken the observables should approach their physical values. The question of renormalization is intimately related to the removal of the regulator and prediction of physical observables.

Next the $a \rightarrow 0$ limit is taken analytically in Eq. (12) and then we turn to the question of renormalization. With the present regularization procedure one has for the lattice-renormalized t matrix

$$T_R(k, \lambda_R(\mathcal{A}), \mathcal{A}) = [\lambda_R^{-1}(\mathcal{A}) - \mathcal{I}_R(k, \mathcal{A})]^{-1}, \quad (19)$$

with

$$\mathcal{I}_R(k, \mathcal{A}) = \lim_{a \rightarrow 0} [I_R(k, a) - I_R(i/\mathcal{A}, a)], \quad (20)$$

$$\lambda_R^{-1}(\mathcal{A}) = \lim_{a \rightarrow 0} [\lambda^{-1}(a) - I_R(i/\mathcal{A}, a)], \quad (21)$$

where \mathcal{A} is the lattice-renormalization scale of the problem. This scale \mathcal{A} should be contrasted with the physical scale Λ_0 of Eqs. (17) and (18). In Eq. (19) the explicit dependence of the t matrix on both \mathcal{A} and the lattice-renormalized coupling $\lambda_R(\mathcal{A})$ has been exhibited.

After taking the $a \rightarrow 0$ limit in Eq. (20) and using Eq. (8), the following lattice-renormalized function is obtained

$$\begin{aligned} \mathcal{I}_R(k, \mathcal{A}) &= \lim_{a \rightarrow 0} a^{(2-\mathcal{D})} \left(\prod_{l=1}^{\mathcal{D}} \int_{-\pi}^{\pi} \frac{d\tilde{q}_l}{(2\pi)^3} \right) \\ &\times \frac{-a^2(\mathcal{A}^{-2} + k^2)}{[\{a^2 k^2 - 2\mathcal{D} + \sum_{j=1}^{\mathcal{D}} 2 \cos \tilde{q}_j + i0\}[-a^2/\mathcal{A}^2 - 2\mathcal{D} + \sum_{j=1}^{\mathcal{D}} 2 \cos \tilde{q}_j]]} \\ &= \int d^{\mathcal{D}} q \frac{\mathcal{A}^{-2} + k^2}{(k^2 - q^2 + i0)(\mathcal{A}^{-2} + q^2)}. \end{aligned} \quad (22)$$

Consequently,

$$\mathcal{I}_R(k, \mathcal{A}) = -2\pi^2(ik + 1/\mathcal{A}), \mathcal{D} = 3, \quad (23)$$

$$\mathcal{I}_R(k, \mathcal{A}) = 2\pi \ln(k\mathcal{A}) - i\pi^2, \mathcal{D} = 2, \quad (24)$$

In Eq. (21), if integrals I_R are evaluated and the trivial limit $a \rightarrow 0$ taken, we get

$$\lambda_R(\mathcal{A}) = -[2\pi^2/\mathcal{A} + 2\pi^2\Lambda_0]^{-1}, \mathcal{D} = 3, \quad (25)$$

$$= [2\pi \ln(\mathcal{A}\Lambda_0)]^{-1}, \mathcal{D} = 2. \quad (26)$$

The lattice-renormalized coupling for two scales \mathcal{A} and \mathcal{A}_0 are related by the flow equations:

$$\lambda_R^{-1}(\mathcal{A}) + 2\pi^2/\mathcal{A} = \lambda_R^{-1}(\mathcal{A}_0) + 2\pi^2/\mathcal{A}_0, \quad (27)$$

$$\lambda_R^{-1}(\mathcal{A}) - 2\pi \ln \mathcal{A} = \lambda_R^{-1}(\mathcal{A}_0) - 2\pi \ln \mathcal{A}_0, \quad (28)$$

for $\mathcal{D} = 3$ and 2, respectively. The flow equations are independent of the renormalization scheme.

The present scattering model permits analytic solution and for $\mathcal{D} = 3$ and 2 the exact lattice-renormalized t matrices of Eq. (19) are given, respectively, by

$$T_R(k, \lambda_R(\mathcal{A}), \mathcal{A}) = [\lambda_R^{-1}(\mathcal{A}) + 2\pi^2(1/\mathcal{A} + ik)]^{-1}, \quad (29)$$

$$= [\lambda_R^{-1}(\mathcal{A}) - 2\pi \ln(k\mathcal{A}) + i\pi^2]^{-1}. \quad (30)$$

Explicitly, using definitions (25) and (26) for the renormalized coupling, these lattice-renormalized t matrices can be written as

$$T_R(k, \lambda_R(\mathcal{A}), \mathcal{A}) = [2\pi^2(ik - \Lambda_0)]^{-1}, \mathcal{D} = 3 \quad (31)$$

$$= [-2\pi \ln(k/\Lambda_0) + i\pi^2]^{-1}, \mathcal{D} = 2. \quad (32)$$

These t matrices depend on $\lambda_R(\mathcal{A})$, but not on \mathcal{A} , that is the explicit and implicit (through $\lambda_R(\mathcal{A})$) dependences of the t matrix on \mathcal{A} cancel. Physics is determined by the value of $\lambda_R(\mathcal{A})$ at an arbitrary value of \mathcal{A} [8]. For $\mathcal{D} = 3$, the physical scale Λ_0 is related to the scattering length a_0 by $a_0 = -1/\Lambda_0$. For $\mathcal{D} = 2$, Λ_0 can also be related to the scattering length [10].

Next we write the RG equation for this problem and show how the limit $a \rightarrow 0$ can be taken numerically. In this limit the lattice-renormalized t matrix is independent of a , so is invariant under the group of transformations $a \rightarrow \exp(s)a$, which form the RG. It is convenient to work in terms of the dimensionless coupling, $g(a)$, defined by

$$g(a) \equiv c\lambda(a)/a, \mathcal{D} = 3, \quad (33)$$

$$\equiv 2\pi\lambda(a), \mathcal{D} = 2. \quad (34)$$

The renormalization condition in the $a \rightarrow 0$ limit can be expressed as [1]

$$a \frac{d}{da} T(k, g(a), a) = 0, \quad (35)$$

or,

$$\left[a \frac{\partial}{\partial a} + \beta(g) \frac{\partial}{\partial g} \right] T(k, g(a), a) = 0, \quad (36)$$

where the RG function $\beta(g)$ is defined by

$$\beta(g) = a \frac{\partial g(a)}{\partial a}. \quad (37)$$

Equation (36) is the RG equation. As the present problem permits analytic solution, the constant $\beta(g)$ of Eq. (37) can be exactly calculated.

For both $\mathcal{D} = 3$, and 2, $\beta(g)$ is a finite quantity independent of a . For $\mathcal{D} = 3$, from Eqs. (17), (33) and (37) we have $\beta(g) = -g - g^2$. Similarly, for $\mathcal{D} = 2$, from Eqs. (18), (34), and (37) we have $\beta(g) = -g^2$.

One has the following Taylor series relating the solution for a small finite a , and that for $a \rightarrow 0$:

$$T(k, a) = T(k, 0) + \frac{a^2}{2!} T''(k, 0) + \frac{a^3}{3!} T'''(k, 0) \dots,$$

where prime(s) denote derivative with respect to a at $a = 0$. Here the linear term in a does not contribute, as the RG equation (35) yields $T'(k, 0) = 0$. Though the first order derivative is zero by the RG equation, the higher-order derivatives are not zero. Then the converged, $a \rightarrow 0$, result is given, approximately, by

$$T(k, 0) \approx T(k, a) - \frac{a^2}{2!} T''(k, a) - \frac{a^3}{3!} T'''(k, a) \dots, \quad (38)$$

where the derivatives are to be calculated for a small finite a . For evaluating T'' (T''') numerically one needs $T(k, a)$ for three (four) adjacent values of a . As more terms are maintained in Eq. (38) a more converged $a \rightarrow 0$ limit is obtained.

In summary, we have used the lattice technique for solving the nonrelativistic quantum scattering problem with delta potential in two and three dimensions. This technique leads to a lattice-regularized Green function. Finite physical result is obtained by employing standard renormalization procedure with this regularized Green function as the continuum limit is taken. The RG equation is written for this problem. Lattice technique and RG equation should be valid for general nonrelativistic potential models with ultraviolet divergence. Though we have illustrated the lattice technique for scattering problems with ultraviolet divergences, it should be applicable to any scattering problem. In fact, the present study strongly suggests that, as in QED and QCD, with the use of modern computers the lattice technique should be a powerful alternative tool for the numerical solution of general nonrelativistic few- and many-body problems, where, unlike in the present delta potential problems, analytic solutions can not be formulated.

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